Semiempirical Models of Shear Modulus at Shock Temperatures and Pressures

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Numerical modeling of the elastic-plastic flow of shocked material requires models which describe the temperature and baric behavior of shear modulus. The paper systematically compares a number of such models in their ability to reproduce experimental and calculated (ab initio) data at temperatures and pressures typical of solid states behind the shock front. We considered two widely used models: the Steinberg-Cochran-Guinan (*SCG*) model [1] and the Burakovsky-Preston (*BP*) model [2,3], as well as the (*V*,*T*)-model proposed in [4].

The *SCG* model is based on a liner representation of shear modulus as a function of temperature *T* and pressure *P* (low pressures) with account for its asymptotic behavior at ultrahigh compressions:

$$\mu(P,T) = \mu_{300} + \mu'_P \times P \times x^{1/3} + \mu'_T \times (T - 300),$$

where $x = V / V_{300}$, *V* is molar volume; μ_{300} and V_{300} are values of shear modulus and molar volume at *T*=300K and *P*=0; and μ'_P, μ'_T are pressure and temperature derivatives of shear modulus.

In the *BP* model, shear modulus is written as a sum of cold and thermal components. The analytical representation of the cold component is based on the relation between shear modulus and Debye temperature and hence the Gruneisen function written as $\gamma(\rho) = \frac{1}{2} + \gamma_1 X^{1/3} + \gamma_2 X^q$, where γ_1, γ_2, q are model parameters, $X = \rho_{00}/\rho$, ρ_{00} is density at *T*=0 and *P*=0. As the *SCG* model, the *BP* one correctly describes the asymptotic behavior of shear modulus. Shear modulus finally takes the form

$$\mu(\rho,T) = \mu_{00} X^{-4/3} \exp\left[6\gamma_1\left(1 - X^{1/3}\right) + \frac{2\gamma_2}{q}\left(1 - X^q\right)\right] - a\rho T .$$

In the (*V*,*T*)-model, shear modulus is proposed to be written as

$$\mu(V,T) = \mu_{00} + \mu'_P \times P_C(X) \times X^a - \frac{g_z E_T(V,T)}{V},$$

where $X=V/V_{00}$, V_{00} and μ_{00} are molar volume and shear modulus at $T = 0$ and $P = 0$, $P_C(X)$ is cold pressure (compression isotherm), E_T is thermal energy, and g_z is a shear analog of the Gruneisen parameter. Thermal energy can be taken either in the form used in the Debye model, $E_T = 3RT \times D(t_D)$, or in that used in the Einstein model, $E_T = 3RTt_E\left[\exp(t_E) - 1\right]^{-1}$. Here $D(t)$ is Debye function, $t_{D,E} = \frac{q_{D,E}(V)}{T}$, q_D and q_E are characteristic temperatures in Debye and Einstein models. In both cases, shear modulus at high temperatures is defined by

$$\mu(V,T) = \mu_{00} + \mu_P' \times P_C(X) \times X^{a} - 3\frac{\gamma_z RT}{V}.$$

The cold part of the (V,T)-model is close in form to the *SCG* model at $T = 0$, but it includes a free parameter a which allows accounting for specific materials. It is shown that data from First Principles (FP) calculations are well reproduced for most metals when a takes values between 1 and 2 which are much higher than 1/3 used in the *SCG* model.

Our comparison of the three models, which was done for 10 metals (*Al, Be, Cu, K, Na, Mg, Mo, W, Ta, U*) shows that the functional representation of the (V,T)- and *BP*-models with appropriately chosen parameters allows a consistent description of FP calculations in a wide range of compressions and experimental values of shear modulus and its baric derivative at $P = 0$. For *Al, Cu, Mo, W* and *Ta* we also managed to adequately reproduce experimental data on temperature dependent shear moduli and longitudinal sound velocities behind the shock front. It is shown that parameters of the *BP* model in this case strongly differ from those proposed in [2,3]. In comparison with FP results, the *SCG* model often overestimates shear modulus as pressure grows. This is also due to the fact that the model is capable of treating the asymptotic behavior. Thus the factors responsible for the asymptotic behavior do not yet dominate at high interim pressures typical of shock compression.

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